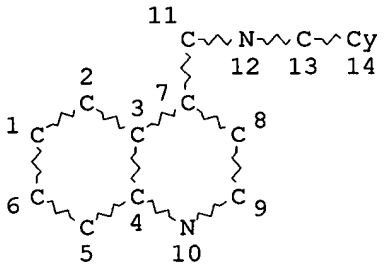
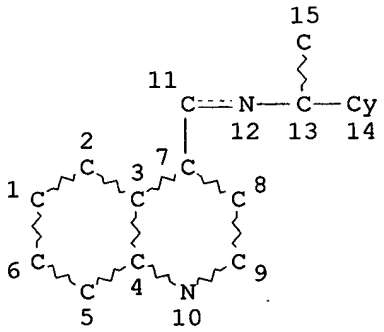
Mullis
450437


```
=> fil reg; d que stat; fil ca,caplus; s l5 or l5/d
FILE 'REGISTRY' ENTERED AT 11:13:41 ON 17 JUN 1997
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 1997 American Chemical Society (ACS)

STRUCTURE FILE UPDATES:  15 JUNE 97  HIGHEST RN 189933-40-2
DICTIONARY FILE UPDATES: 16 JUNE 97  HIGHEST RN 189933-39-9

TSCA INFORMATION NOW CURRENT THROUGH DECEMBER 1996

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.


L1              STR
```




```
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  14

STEREO ATTRIBUTES: NONE
L2          194 SEA FILE=REGISTRY SSS FUL L1
L4              STR
```




```
NODE ATTRIBUTES:
NSPEC   IS RC     AT  15
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
```

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
L5 120 SEA FILE=REGISTRY SUB=L2 SSS FUL L4

100.0% PROCESSED 192 ITERATIONS 120 ANSWERS
SEARCH TIME: 00.00.03

FILE 'CA' ENTERED AT 11:13:42 ON 17 JUN 1997
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE 'CAPLUS' ENTERED AT 11:13:42 ON 17 JUN 1997
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

L6 10 FILE CA
L7 11 FILE CAPLUS

TOTAL FOR ALL FILES
L8 21 L5 OR L5/D

=> dup rem l8; d 1-11 .bevstr; sel hit l7 1-11 rn
PROCESSING COMPLETED FOR L8
L9 11 DUP REM L8 (10 DUPLICATES REMOVED)

L9 ANSWER 1 OF 11 CAPLUS COPYRIGHT 1997 ACS
AN 1997:320920 CAPLUS
TI Discovery of a Novel Class of Selective Non-Peptide Antagonists for the Human Neurokinin-3 Receptor. 1. Identification of the 4-Quinolinecarboxamide Framework
AU Giardina, Giuseppe A. M.; Sarau, Henry M.; Farina, Carlo; Medhurst, Andrew D.; Grugni, Mario; Raveglia, Luca F.; Schmidt, Dulcie B.; Rigolio, Roberto; Luttmann, Mark; Vecchietti, Vittorio; Hay, Douglas W. P.
CS Department of Chemistry, SmithKline Beecham S.p.A., Baranzate, 20021, Italy
SO J. Med. Chem. (1997), 40(12), 1794-1807
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB A novel class of potent and selective non-peptide neurokinin-3 (NK-3) receptor antagonists, featuring the 4-quinolinecarboxamide framework, was designed based upon chem. diverse NK-1 receptor antagonists. The novel compds., prompted by chem. modifications of the prototype, were characterized by binding anal. using a membrane prepn. of chinese hamster ovary (CHO) cells expressing the human neurokinin-3 receptors (hNK-3-CHO), and clear structure-activity relationships (SARs) were established. From SARs, (R)-N-[.alpha.-(methoxycarbonyl)benzyl]-2-phenylquinoline-4-carboxamide (I, SB 218795, hNK-3-CHO binding Ki = 13 nM) emerged as one of the most potent compds. of this novel class. Selectivity studies vs. the other neurokinin receptors (hNK-2-CHO and hNK-1-CHO)

revealed that 65 is about 90-fold selective for hNK-3 vs. hNK-2 receptors (hNK-2-CHO binding Ki = 1221 nM) and over 7000-fold selective vs. hNK-1 receptors (hNK-1-CHO binding Ki = >100 .mu.M). In vitro functional studies in rabbit isolated iris sphincter muscle prepn. demonstrated that I a competitive antagonist of the contractile response induced by the potent and selective NK-3 receptor agonist senktide with a Kb = 43 nM. Overall, the data indicate that I is a potent and selective hNK-3 receptor antagonist and a useful lead for further chem. optimization.

IT RN LIST MAY NOT BE COMPLETE: 67-64-1 70-11-1 75-05-8 83-93-2 88-15-3 91-56-5 93-98-1 94-02-0 98-86-2 99-02-5 99-91-2 99-93-4 100-06-1 102-04-5 103-79-7 118-93-4 122-00-9 132-60-5 445-27-2 451-40-1 529-34-0 577-16-2 579-74-8 823-76-7 826-73-3 1072-82-8 1072-83-9 1122-54-9 1192-62-7 1468-83-3 1646-26-0 1647-89-8 1721-96-6 2142-68-9 3446-58-0 4364-02-7 4637-24-5 4903-36-0 5466-31-9 6952-34-7 7672-01-7 13226-98-7 14228-23-0 20146-23-0 20146-25-2 20389-05-3 20389-09-7 20389-10-0 20389-11-1 20662-89-9 21908-20-3 24295-03-2 31792-47-9 52351-75-4 55240-51-2 73178-52-6 92566-43-3 92566-45-5 92566-89-7 111588-91-1 **174635-51-9** **174635-52-0** **174635-53-1** **174635-54-2** **174635-56-4** **174635-58-6** **174635-59-7** **174635-60-0** **174635-61-1** 174635-67-7 **174635-71-3** **174635-73-5** **174635-91-7** **174635-97-3** **174635-98-4** 174635-99-5 **174636-00-1** **174636-01-2** **174636-04-5** **174636-06-7** **174636-07-8** **174636-09-0** **174636-13-6** **174636-23-8** **174636-24-9** **174636-25-0** **174636-40-9** 174636-63-6 174636-64-7 174636-84-1 174636-85-2 174636-88-5 174636-91-0 177360-18-8 177360-23-5 177360-24-6 177360-26-8 177360-27-9 177360-30-4 177360-31-5 177360-32-6 177606-27-8 181048-49-7 189815-81-4 189815-82-5 189815-86-9 189815-87-0 **189815-88-1** 189815-92-7 **189815-93-8** **189815-94-9** 189815-95-0 189815-96-1 189815-97-2 189815-98-3 189815-99-4 189816-00-0 189816-01-1 189816-02-2 189816-03-3 189816-04-4 189816-05-5 189816-06-6

L9 ANSWER 2 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 1
AN 126:89156 CA
TI Preparation of chiral isothioyanates as derivatizing agents
IN Lindner, Wolfgang; Kleidernigg, Oliver Paul
PA Lindner, Wolfgang, Austria; Kleidernigg, Oliver Paul
SO PCT Int. Appl., 42 pp.
CODEN: PIXXD2
PI WO 9637465 A1 961128
DS W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE
AI WO 96-EP2258 960524
PRAI EP 95-108125 950526
DT Patent
LA English
OS MARPAT 126:89156
AB R1NHCHR2CHR3NCS [R1 = COR4, CO2R5, SO2R6; R2,R3 = aliph. or arom. group; R2R3 = atoms to complete carbocyclic or heterocyclic ring; R4

= aliph. or (hetero)arom. group, aralkyl; R5 = CMe3, (nitro)benzyl, fluorenylmethyl; R6 = (hetero)aryl] were prepd. Thus, (R,R)-1,2-diaminocyclohexane was cyclocondensed with CS2 and the product amidated by 3,5-(O2N)2C6H3COCl to give (R,R)-N-(2-isothiocyanatocyclohexyl)-3,5-dinitrobenzamide. The latter was used to prep. diastereomeric derivs. of (R)-, and (S)-propranolol. Data for chromatog. sepns. of, e.g., amino acids, etc. were given.

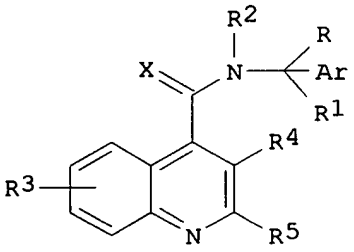
IT **185508-91-2P 185508-92-3P**
RL: NUU (Nonbiological use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of chiral isothiocyanates as derivatizing agents)

L9 ANSWER 3 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 2
AN 125:25636 CA
TI 2-Phenyl-4-quinolinecarboxamides: A Novel Class of Potent and Selective Non-Peptide Competitive Antagonists for the Human Neurokinin-3 Receptor
AU Giardina, Giuseppe A. M.; Sarau, Henry M.; Farina, Carlo; Medhurst, Andrew D.; Grugni, Mario; Foley, James J.; Raveglia, Luca F.; Schmidt, Dulcie B.; Rigolio, Roberto; et al.
CS Department of Chemistry, SmithKline Beecham S.p.A., Baranzate, 20021, Italy
SO J. Med. Chem. (1996), 39(12), 2281-2284
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CJACS-IMAGE; CJACS
AB A novel class of potent and selective, non-peptide NK-3 receptor antagonists, based on the 2-phenylquinoline framework, has been identified and characterized by binding anal. using membrane prepn. of CHO cells expressing the human neurokinin receptors (hNKs-CHO). Functional activity was detd. by inhibition of senktide-induced contraction of the rabbit isolated iris sphincter muscle prepn. An extensive structure-activity study led to the identification of (S)-(-)-N-(.alpha.-ethylbenzyl)-3-hydroxy-2-phenylquinoline-4-carboxamide (SB 223412) as the most potent (Ki = 1.0 nm in hNK-3-CHO binding; Kb = 5.4 nM for antagonism of senktide-induced contraction in rabbit iris sphincter muscle) and selective (hNK-2/hNK-3 Ki ratio of 144 and hNK-1/hNK-3 Ki ratio > 100,000) hNK-3 receptor antagonist of this class. In addn., NKB-induced Ca2+ mobilization studies in hNK-3-HEK 293 cells indicated that SB 223412 is a reversible, competitive antagonist. Compds. from this novel class will be extremely useful in the functional characterization of hNK-3 receptors and elucidation of potential therapeutic indications for selective hNK-3 receptor antagonists.

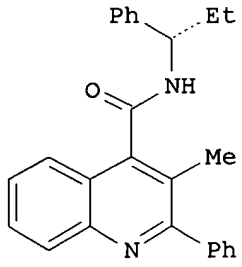
IT **174635-51-9P 174635-52-0P 174635-53-1P**
174635-69-9P 174636-20-5P 174636-32-9P,
SB 223412
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and structure-activity of human neurokinin 3 receptor antagonists phenylquinolinecarboxamides)

L9 ANSWER 4 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 3
AN 124:232269 CA
TI Quinoline derivatives as tachykinin NK3 receptor antagonists
IN Farina, Carlo; Giardina, Giuseppe Arnaldo Mari; Grugni, Mario; Raveglia, Luca Francesco
PA Smithkline Beecham Farmaceutici S.P.A., Italy
SO PCT Int. Appl., 95 pp.

CODEN: PIXXD2
PI WO 9532948 A1 951207
DS W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG
AI WO 95-EP2000 950523
PRAI IT 94-MI1099 940527
IT 95-MI494 950314
DT Patent
LA English
OS MARPAT 124:232269
GI



I



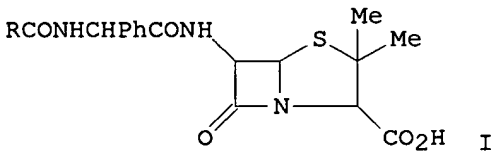
II

AB NK3 receptor antagonists I [Ar = (un)substituted Ph, naphthyl, cycloalkadienyl, heteroaryl; R = (un)substituted alkyl, cycloalkyl, (un)substituted Ph, phenylalkyl, or heteroaryl, CO2H and derivs., etc.; R1, R2 = H, alkyl; or R1R2 = (CH2)3-5; or RR1 = (CH2)2-5; R3, R4 = H, alkyl, alkenyl, aryl, alkoxy, OH, halo, NO2, amino, etc.; R5 = alkyl, cycloalkyl, (un)substituted (hetero)aryl; X = O, S, N(CN)] are useful in treating pulmonary, CNS, and neurodegenerative disorders, etc. Approx. 115 compds. were prepd. For example, amidation of 3-methyl-2-phenylquinoline-4-carbonyl chloride with (R)-.alpha.-ethylbenzylamine gave title compd. II in 58% yield. II had IC50 of 5.6 nM for displacement of [3H]-senktide from guinea-pig cortical NK3 receptors. Antagonist activity of I was shown by inhibition of senktide-induced contraction of guinea-pig ileum.

IT **174635-48-4P 174635-49-5P 174635-50-8P**
174635-51-9P 174635-52-0P 174635-53-1P
174635-54-2P 174635-55-3P 174635-56-4P
174635-57-5P 174635-58-6P 174635-59-7P
174635-60-0P 174635-61-1P 174635-62-2P
174635-63-3P 174635-64-4P 174635-65-5P
174635-66-6P 174635-68-8P 174635-69-9P
174635-70-2P 174635-71-3P 174635-72-4P
174635-73-5P 174635-74-6P 174635-75-7P
174635-76-8P 174635-77-9P 174635-78-0P
174635-79-1P 174635-80-4P 174635-81-5P
174635-82-6P 174635-83-7P 174635-84-8P
174635-85-9P 174635-86-0P 174635-87-1P
174635-88-2P 174635-89-3P 174635-90-6P
174635-91-7P 174635-92-8P 174635-93-9P
174635-94-0P 174635-95-1P 174635-96-2P

174635-97-3P 174635-98-4P 174636-00-1P
174636-01-2P 174636-03-4P 174636-04-5P
174636-05-6P 174636-06-7P 174636-07-8P
174636-09-0P 174636-10-3P 174636-11-4P
174636-12-5P 174636-13-6P 174636-14-7P
174636-15-8P 174636-16-9P 174636-17-0P
174636-18-1P 174636-19-2P 174636-20-5P
174636-21-6P 174636-22-7P 174636-23-8P
174636-24-9P 174636-25-0P 174636-26-1P
174636-27-2P 174636-28-3P 174636-29-4P
174636-30-7P 174636-31-8P 174636-32-9P
174636-33-0P 174636-34-1P 174636-35-2P
174636-36-3P 174636-37-4P 174636-38-5P
174636-39-6P 174636-40-9P 174636-41-0P
174636-42-1P 174636-43-2P 174636-44-3P
174636-45-4P 174636-46-5P 174636-47-6P
174636-48-7P 174636-49-8P 174636-50-1P
174636-51-2P 174636-52-3P 174636-53-4P
174636-54-5P 174636-55-6P 174636-56-7P
174636-57-8P 174636-58-9P 174636-59-0P
174636-60-3P 174636-61-4P 174636-62-5P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of quinolinecarboxamide derivs. as tachykinin NK3 receptor antagonists)

L9 ANSWER 5 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 4
AN 93:186338 CA
TI Ampicillin derivatives
PA Mitsubishi Yuka Yakuhin Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
PI JP 55055194 800422 Showa
AI JP 78-127324 781018
DT Patent
LA Japanese
GI

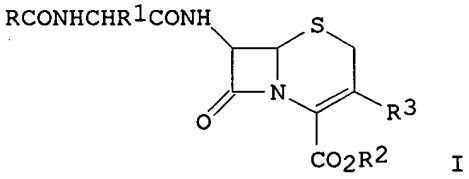


I

AB Fifteen title derivs. I (R = heterocyclic, heterocyclic-substituted methyl) were prepd. and the min. inhibition concns. treated against Ps. aeruginosa, St. aureus, B. substilis, E. coli, Kl. pneumoniae, and Pr. vulgaris. Thus, 618 mg DCC was added to a mixt. of 648 4-carbamoyl-2-quinolinecarboxylic acid and 345 mg N-hydroxysuccinimide in DMF with ice cooling, the mixt. stirred 10 h with ice cooling, a mixt. of 1.2 g ampicillin-3H2O and 0.42 mL Et3N in CH2Cl2-DMF added, and the mixt. stirred 3 h at room temp. to give, after treating with K 2-ethylhexanoate, 1.32 d-I (R = 4-carbamoyl-2-quinolyl) K salt.
IT **75204-90-9P**

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and bactericidal activity of)

L9 ANSWER 6 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 5
AN 90:38949 CA
TI Cephalosporins with .alpha.-acylaminoacetic acid side chains
IN Kocsis, Karoly; Peter, Heinrich; Bickel, Hans
PA Ciba-Geigy A.-G., Switz.
SO Swiss, 11 pp.
CODEN: SWXXAS
PI CH 606006 781013
AI CH 74-6494 740513
DT Patent
LA German
GI

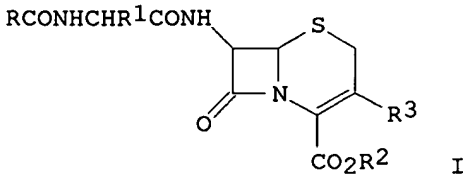


I

AB The cephalosporins I [R = 6-membered ring contg. 1-3 N atoms and an oxo group (optionally substituted or condensed with other rings); R1 = (substituted) Ph, thienyl, furyl, cyclohexadienyl; R2 = H, ester group; R3 = H, alkoxy, substituted Me] were prepd. for use as bactericides, e.g., at 8-100 mg/kg s.c. in mice against Staphylococcus aureus. Thus, D-(-)-(1,6-dihydro-6-oxo-3-pyridazinylcarbonylamino)phenylacetic acid reacted with ClCO2Et, N-methylmorpholine, and 7.beta.-aminocephalosporanic acid in THF to give D-7.beta.-I (R = 1,6-dihydro-6-oxo-3-pyridazinyl, R1 = Ph, R2 = H, R3 = AcOCH2).

IT **59133-55-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 7 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 6
AN 90:38951 CA
TI Cephalosporins with .alpha.-acylaminoacetic acid side chains
IN Kocsis, Karoly; Peter, Heinrich; Bickel, Hans
PA Ciba-Geigy A.-G., Switz.
SO Swiss, 11 pp.
CODEN: SWXXAS
PI CH 606001 781013
AI CH 74-6494 740513
DT Patent
LA German
GI



I

AB The cephemcarboxylic acids I [R = 6-membered ring contg. 1-3 N atoms and an oxo group, optionally substituted or condensed with other rings; R1 = (substituted) Ph, thienyl, furyl, cyclohexadienyl; R2 = H, physiol. cleavable ester group; R3 = H, (substituted) Me, lower alkoxy] were prepd. for use as bactericides, e.g., at 8-100 mg/kg s.c. against Staphylococcus aureus in mice. Thus, cephaloglycin reacted with 6-hydroxy-3-pyridinecarbonyl chloride in CH2Cl2 to give I (R = 6-hydroxy-3-pyridyl, R1 = Ph, R2 = H, R3 = CH2OAc).

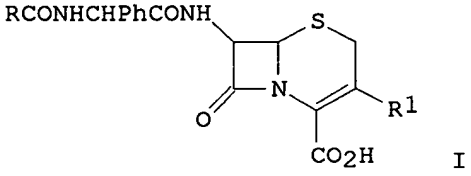
IT **59133-55-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 8 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 7
AN 84:135637 CA
TI Penicillins
IN Tobiki, Hisao; Shimaji, Kozo; Okano, Shigeru; Komatsu, Toshiaki; Katsura, Toyozo; Taira, Yasushi; Eda, Yasuko
PA Sumitomo Chemical Co., Ltd., Japan
SO Japan., 11 pp.
CODEN: JAXXAD
PI JP 50023036 B4 750805 Showa
AI JP 70-124363 701229
DT Patent
LA Japanese
GI For diagram(s), see printed CA Issue.
AB Acids ROH I (Z = O, S; R1 = alkyl, cycloalkylalkyl, alkenyl, aralkyl, OH, alkoxy, aralkyloxy; R2 = H, alkyl; A = benzo, naphtho, pyrido) were treated with 6-aminopenicillanic acid (III) or its derivs. to give II. II are bactericides not only against gram-pos. and -neg. bacteria but also against Pseudomonas aeruginosa (min. inhibitory concn. 3.13-50 .mu.g/ml). Thus, 2 g 1-hydroxy-6,7-methylenedioxy-4-quinolone-3-carboxylic acid in CH2Cl2 was treated with Et3N, 1.8 g ClCO2Et, and 1.65 g D(-)-.alpha.-phenylglycine Et ester-HCl to give 1.8 g D(-)-.alpha.-(1-hydroxy-6,7-methylenedioxy-4-quinolone-3-carboxamido)phenylacetic acid, which (1 g) in CH2Cl2 was treated with Et3N, ClCO2Et and 0.83 g III Et3N salt to give 1.3 g D(-)-II (Z = O, R1 = OH, R2 = H, A = 6,7-methylenedioxybenzo). Among 25 more II prepd. were (Z, R1, R2, A given): O, Et, H, 6-methoxybenzo; O, Me, H, X; O, Et, H, 1,2-naphtho; O, OEt, H, 6,7-methylenedioxybenzo.

IT **58865-82-0P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and bactericidal activity of)

L9 ANSWER 9 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 8
AN 84:164802 CA
TI Cephalosporins with .alpha.-acylaminoacetic acid side chain
IN Kocsis, Karoly; Peter, Heinrich; Bickel, Hans
PA Ciba-Geigy A.-G., Switz.

SO Ger. Offen., 80 pp.
CODEN: GWXXBX
PI DE 2520561 751127
PRAI CH 74-6494 740513
DT Patent
LA German
GI



I

AB Of the cephalosporins I (R = N heterocyclyl, R1 = CH2OAc, OMe, heterocyclic thiomethyl pyridiniomethyl) were prepd. by acetylating cephaloglycines and substituting on acetoxymethyl group. Thus, I (R = 2-hydroxy-5-pyridyl, R1 = OAc) was obtained by treating cephaloglycine with 2-hydroxy-5-pyridinecarbonyl chloride.
IT **59133-55-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 10 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 9
AN 70:47439 CA
TI .alpha.-Amidobenzyl- and amido(2-thienyl)methylpenicillins
IN Long, Anthony Alfred W.; Nayler, John H. C.
PA Beecham Group Ltd.
SO Brit., 6 pp.
CODEN: BRXXAA
PI GB 1130445 681016
AI GB 660426
DT Patent
LA English
GI For diagram(s), see printed CA Issue.
AB The 6-aminopenicillanic acid derivs. prepd. had the structure I, where R is a Ph or thienyl group, R1 is a heterocyclic group, and n is 0 or 1. The compds. were useful as antibacterial agents, as nutritional supplements in animal food, and in the treatment of infectious diseases caused by gram-pos. and gram-neg. bacteria. Thus, a suspension of 12.8 g. D-.alpha.-aminobenzylpenicillin (II) trihydrate in 80 ml. H2O was adjusted to pH 9.2 with 5N aq. NaOH and treated with a soln. of 4.6 g. 5-methyl-3-isoxazolecarbonyl chloride in 100 ml. iso-BuCOMe (III). After stirring for 2 hrs. at room temp., the mixt. was filtered through Dicalite and the layers were sepd. The org. phase was washed with satd. brine and treated with 16 ml. 2N Na 2-ethylhexanoate in III to give 13 g. Na salt of D-.alpha.-(5-methyl-3-iso-xazolecarboxamido)benzylpenicillin which crystd. on trituration with ether. The sodium salts of D-.alpha.-(5-methyl-4-isoxazolecar-boxamido)benzylpenicillin, D-.alpha.-(2-furancarboxamido)benzylpenicillin, D-.alpha.-(3-thiophenecarboxamido)benzylpenicillin, D-.alpha.-(2-thiophenecarboxamido)benzylpenicillin, D-.alpha.-(2-thiopheneacetamido)benzylpenicillin, D-.alpha.-(3-thiopheneacetamido)benzylpenicillin, D-.alpha.-(3-ethoxy-4-quinolinecarboxamido)benzylpenicillin, D-.alpha.-(8-methoxy-2-

quinolinecarboxamido)benzylpenicillin, D-.alpha.-(2-pyridinecarboxamido)benzylpenicillin, D-.alpha.-(phthalimidoacetamido)-benzylpenicillin, D-.alpha.-(2,6-dioxo-4-piperidineacitamido)benzylpenicillin, D-.alpha.-(2-oxo-2H-pyran-5-carboxamido)benzylpenicillin, D-.alpha.-(5-methyl-3-phenyl-4-isoxazolecarboxamido)benzylpenicillin, D-.alpha.-(3-methyl-5-phenyl-4-isoxazolecarboxamido)benzylpenicillin, D-.alpha.-(5-bromo-2-(methylthio)-4-pyrimidinecarboxamido)benzylpenicillin, D-.alpha.-(2-furoylamino)-2-thienylmethylpenicillin, D-.alpha.-nicotinamidobenzylpenicillin, D-.alpha.-(2-thiopheneacetamido)-2-thi-enylmethylpenicillin, and D-.alpha.-(2-furanacetamido)benzylpenicillin were similarly prepd.

IT **21611-82-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L9 ANSWER 11 OF 11 CA COPYRIGHT 1997 ACS DUPLICATE 10
AN 74:87972 CA
TI Antibacterial acylated benzylpenicillin and thienylmethylpenicillin derivatives
PA Beecham Group Ltd.
SO Fr. M., 4 pp.
CODEN: FMXXAJ
PI FR 6212 680902
PRAI GB 660426
DT Patent
LA French
GI For diagram(s), see printed CA Issue.
AB [.alpha.-(Amino)arylacetamido]penicillin deriv. (I), where Ar is Ph or 2-thienyl, are treated with Ar1(CH2)nCOCl (Ar1 = heteroaryl) to give penicillin diamide derivs. (II). II (n = 0 or 1 and Ar1 is furyl, thienyl, phthalimido, or a substituted quinolyl, piperidyl, oxopyranyl, or isoxazolyl group) are prepd.

IT **21611-82-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

E1 THROUGH E120 ASSIGNED

=> fil reg
FILE 'REGISTRY' ENTERED AT 11:14:19 ON 17 JUN 1997
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 1997 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 15 JUNE 97 HIGHEST RN 189933-40-2
DICTIONARY FILE UPDATES: 16 JUNE 97 HIGHEST RN 189933-39-9

TSCA INFORMATION NOW CURRENT THROUGH DECEMBER 1996

Please note that search-term pricing does apply when conducting SmartSELECT searches.

=> d que
L10 120 SEA FILE=REGISTRY ABB=ON PLU=ON (174635-51-9/BI OR 174635-52-0/BI OR 174635-53-1/BI OR 59133-55-0/BI OR 174635-54-2/BI OR 174635-56-4/BI OR 174635-58-6/BI OR 174635-59-7/BI OR 174635-60-0/BI OR 174635-61-1/BI OR 174635-69-9/BI OR 174635-71-3/BI OR 174635-73-5/BI OR 174635-91-7/BI OR

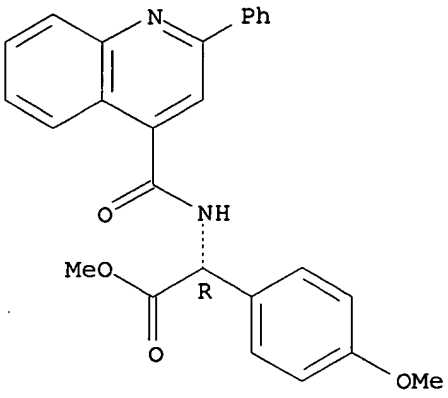
174635-97-3/BI OR 174635-98-4/BI OR 174636-00-1/BI OR 17
4636-01-2/BI OR 174636-04-5/BI OR 174636-06-7/BI OR 17463
6-07-8/BI OR 174636-09-0/BI OR 174636-13-6/BI OR 174636-2
0-5/BI OR 174636-23-8/BI OR 174636-24-9/BI OR 174636-25-0
/BI OR 174636-32-9/BI OR 174636-40-9/BI OR 21611-82-5/BI
OR 174635-48-4/BI OR 174635-49-5/BI OR 174635-50-8/BI OR
174635-55-3/BI OR 174635-57-5/BI OR 174635-62-2/BI OR 174
635-63-3/BI OR 174635-64-4/BI OR 174635-65-5/BI OR 174635
-66-6/BI OR 174635-68-8/BI OR 174635-70-2/BI OR 174635-72
-4/BI OR 174635-74-6/BI OR 174635-75-7/BI OR 174635-76-8/
BI OR 174635-77-9/BI OR 174635-78-0/BI OR 174635-79-1/BI
OR 174635-80-4/BI OR 174635-81-5/BI OR 174635-82-6/BI OR
174635-83-7/BI OR 174635-84-8/BI OR 174635-85-9/BI OR 174
635-86-0/BI OR 174635-87-1/BI OR 174635-88-2/BI OR 174635
-89-3/BI OR 174635-90-6/BI OR 174635-92-8/BI OR 174635-93
-9/BI OR 174635-94-0/BI OR 174635-95-1/BI OR 174635-96-2/
BI OR 174636-03-4/BI OR 174636-05-6/BI OR 174636-10-3/BI
OR 174636-11-4/BI OR 174636-12-5/BI OR 174636-14-7/BI OR
174636-15-8/BI OR 174636-16-9/BI OR 174636-17-0/BI OR 174
636-18-1/BI OR 174636-19-2/BI OR 174636-21-6/BI OR 174636
-22-7/BI OR 174636-26-1/BI OR 174636-27-2/BI OR 174636-28
-3/BI OR 174636-29-4/BI OR 174636-30-7/BI OR 174636-31-8/
BI OR 174636-33-0/BI OR 174636-34-1/BI OR 174636-35-2/BI
OR 174636-36-3/BI OR 174636-37-4/BI OR 174636-38-5/BI OR
174636-39-6/BI OR 174636-41-0/BI OR 174636-42-1/BI OR 174
636-43-2/BI OR 174636-44-3/BI OR 174636-45-4/BI OR 174636
-46-5/BI OR 174636-47-6/BI OR 174636-48-7/BI OR 174636-49
-8/BI OR 174636-50-1/BI OR 174636-51-2/BI OR 174636-52-3/
BI OR 174636-53-4/BI OR 174636-54-5/BI OR 174636-55-6/BI
OR 174636-56-7/BI OR 174636-57-8/BI OR 174636-58-9/BI OR
174636-59-0/BI OR 174636-60-3/BI OR 174636-61-4/BI OR 174
636-62-5/BI OR 185508-91-2/BI OR 185508-92-3/BI OR 189815
-88-1/BI OR 189815-93-8/BI OR 189815-94-9/BI OR 58865-82-
0/BI OR 75204-90-9/BI)

Random RNs/ Strs displayed

=> d 1,4,6,67,117-120 ide; fil caold

L10 ANSWER 1 OF 120 REGISTRY COPYRIGHT 1997 ACS
RN **189815-94-9** REGISTRY
CN INDEX NAME NOT YET ASSIGNED
FS 3D CONCORD; STEREOSEARCH
MF C26 H22 N2 O4
SR CA
LC STN Files: CAPLUS

Absolute stereochemistry.

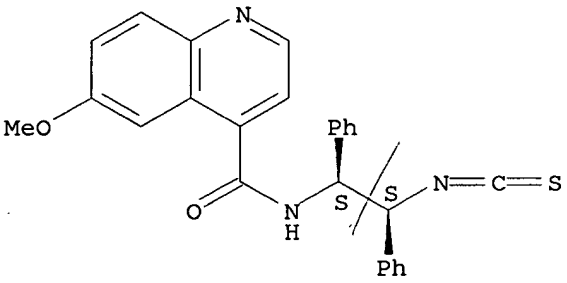


1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L10 ANSWER 4 OF 120 REGISTRY COPYRIGHT 1997 ACS
RN **185508-92-3** REGISTRY
CN 4-Quinolinecarboxamide, N-(2-isothiocyanato-1,2-diphenylethyl)-6-methoxy-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)
FS 3D CONCORD; STEREOSEARCH
MF C26 H21 N3 O2 S
SR CA
LC STN Files: CA, CAPLUS

L9 2 ans

Absolute stereochemistry.

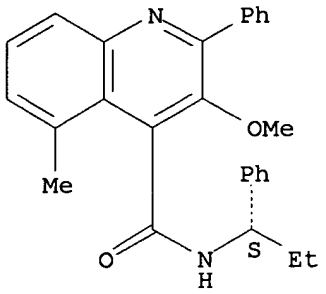


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L10 ANSWER 6 OF 120 REGISTRY COPYRIGHT 1997 ACS
RN **174636-62-5** REGISTRY
CN 4-Quinolinecarboxamide, 3-methoxy-5-methyl-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H26 N2 O2
SR CA
LC STN Files: CA, CAPLUS

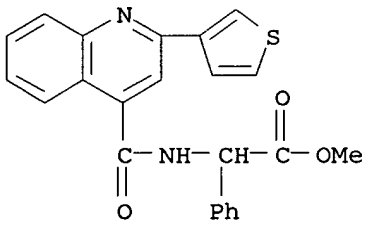
2 hits
PF, appl used

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

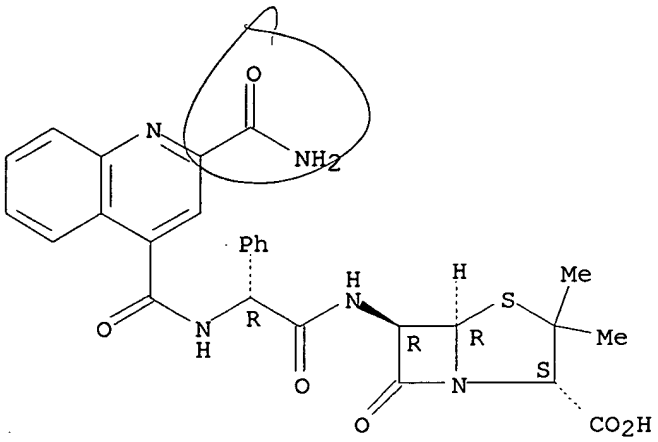
L10 ANSWER 67 OF 120 REGISTRY COPYRIGHT 1997 ACS
RN **174635-98-4** REGISTRY
CN Benzeneacetic acid, .alpha.-[[[2-(3-thienyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H18 N2 O3 S
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L10 ANSWER 117 OF 120 REGISTRY COPYRIGHT 1997 ACS
RN **75204-90-9** REGISTRY
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[2-(aminocarbonyl)-4-quinolinyl]carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, monopotassium salt, [2S-[2.alpha.,5.alpha.,6.beta.(S*)]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H25 N5 O6 S . K
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

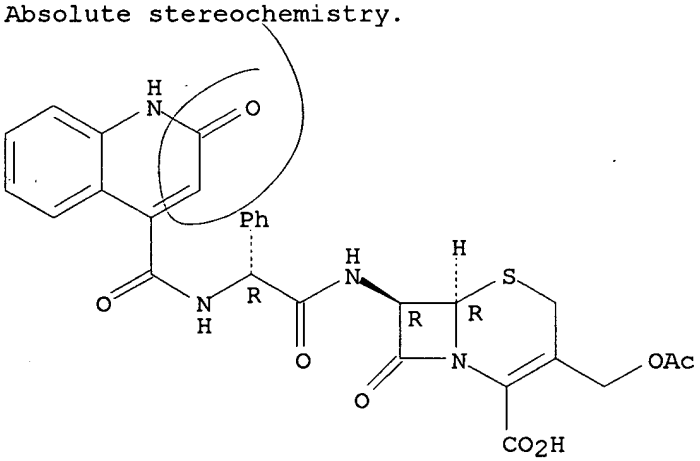


● K

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L10 ANSWER 118 OF 120 REGISTRY COPYRIGHT 1997 ACS
RN **59133-55-0** REGISTRY
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[[(1,2-dihydro-2-oxo-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-8-oxo-, [6R-[6.alpha.,7.beta.(R*)]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C28 H24 N4 O8 S
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Absolute stereochemistry.



3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

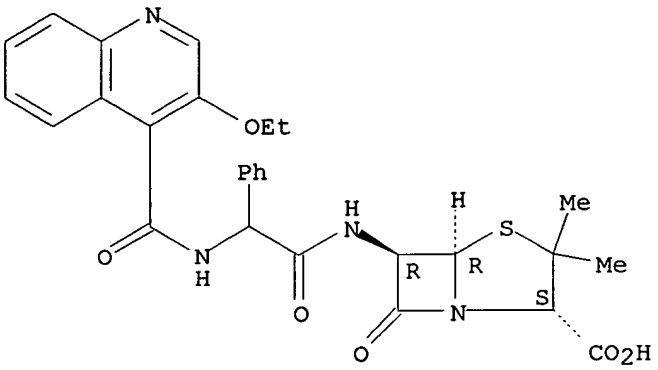
L10 ANSWER 119 OF 120 REGISTRY COPYRIGHT 1997 ACS
RN **58865-82-0** REGISTRY
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[(3-ethoxy-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, monosodium salt, [2S-(2.alpha.,5.alpha.,6.beta.)]-

Searcher : Shears 308-4994

1/4 See new L/8

(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C28 H28 N4 O6 S . Na
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

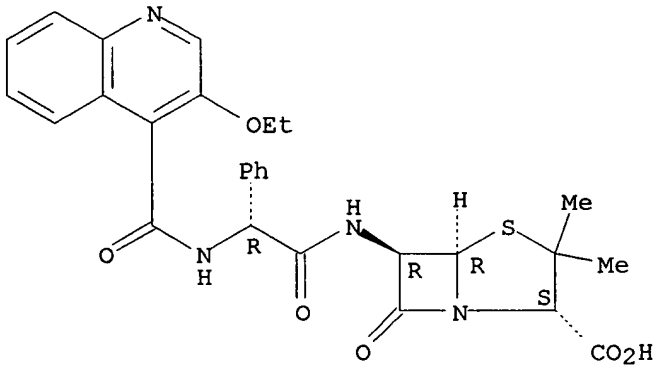


● Na

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L10 ANSWER 120 OF 120 REGISTRY COPYRIGHT 1997 ACS
RN **21611-82-5** REGISTRY
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[2-(3-ethoxycinchoninamido)-2-phenylacetamido]-3,3-dimethyl-7-oxo-, D- (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C28 H28 N4 O6 S
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

FILE 'CAOLD' ENTERED AT 11:16:29 ON 17 JUN 1997
Searcher : Shears 308-4994

FILE COVERS 1957-1966
FILE LAST UPDATED: 30 OCT 91 (910803/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

NEW TO CAOLD: Searchable and selectable accession numbers, hit-term highlighting, and the HITSTR display format. See NEWS for details.

=> s l10
L11 0 L10

=> fil uspat; s l10
FILE 'USPATFULL' ENTERED AT 11:16:41 ON 17 JUN 1997

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 10 Jun 1997 (19970610/PD)
FILE LAST UPDATED: 11 Jun 1997 (970611/ED)
HIGHEST PATENT NUMBER: US5638543
CA INDEXING IS CURRENT THROUGH 11 Jun 1997 (970611/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 10 Jun 1997 (19970610/PD)
REVISED CLASS FIELDS (/NCL) CURRENT THROUGH: APR 1997
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: FEB 1997

>>> Page images are available for patents from 1/1/94. Current <<<
>>> week patent text is typically loaded by Thursday morning and <<<
>>> page images are available for display by the end of the day. <<<
>>> Image data for the /FA field are available the following week. <<<

>>> Complete CA file indexing for chemical patents (or equivalents) <<<
>>> is included in file records. A thesaurus is available for the <<<
>>> USPTO Manual of Classifications in the /NCL, /INCL, and /RPCL <<<
>>> fields. This thesaurus includes catchword terms from the <<<
>>> USPTO/MOC subject headings and subheadings. Thesauri are also <<<
>>> available for the WIPO International Patent Classification <<<
>>> (IPC) Manuals, editions 1-6, in the /IC1, /IC2, /IC3, /IC4, <<<
>>> /IC5, and /IC (/IC6) fields, respectively. The thesauri in <<<
>>> the /IC5 and /IC fields include the corresponding catchword <<<
>>> terms from the IPC subject headings and subheadings. <<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

L12 3 L10

=> d 1-3 bib abs hitstr; fil marpat

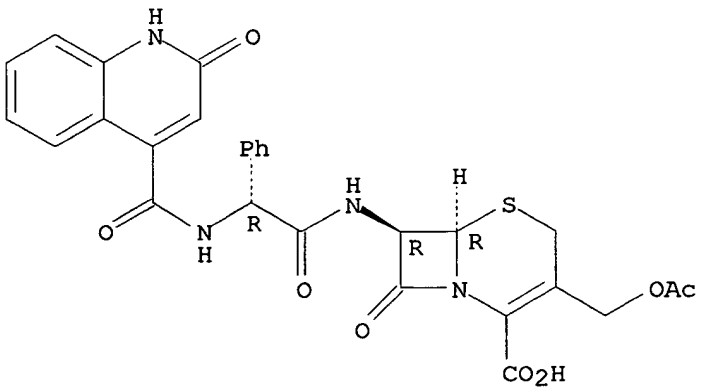
L12 ANSWER 1 OF 3 USPATFULL
AN 81:24739 USPATFULL
TI Cephalosporins having an .alpha.-acylaminoacetic acid side chain
IN Kocsis, Karoly, Basel, Switzerland
Peter, Heinrich, Binningen, Switzerland
Bickel, Hans, Binningen, Switzerland
PA Ciba-Geigy Corporation, Ardsley, NY, United States (U.S.

Searcher : Shears 308-4994

corporation)
PI US 4265892 810505
AI US 79-11359 790212 (6)
RLI Division of Ser. No. US 77-789164, filed on 20 Apr 1977, now patented, Pat. No. US 4154831 which is a division of Ser. No. US 75-576398, filed on 9 May 1975, now patented, Pat. No. US 4041161
PRAI CH 74-6494 740513
DT Utility
EXNAM Primary Examiner: Coughlan, Jr., Paul M.
LREP Almaula, Prabodh I.
CLMN Number of Claims: 10
ECL Exemplary Claim: 1,7
DRWN No Drawings
LN.CNT 1140
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Compounds of the formula ##STR1## wherein R.sub.1 denotes optionally substituted phenyl, thienyl, furyl or 1,4-cyclohexadienyl, R.sub.2 represents a free carboxyl group or an esterified carboxyl group which can be split physiologically, R.sub.3 represents hydrogen, lower alkoxy or an optionally substituted methyl group and B represents an optionally substitued six-membered ring with 1 to 3 ring nitrogen atoms, which is bonded to the carbonyl group --C(.dbd.O)-- by one of its carbon atoms, the nitrogen atoms of a monocyclic six-membered ring having 2 nitrogen atoms being either adjacent or separated by two ring carbon atoms, and the salts of such compounds which have a salt-forming group, including the inner salts, for example the 7.beta.-[D(-)-.alpha.-(3,5-Dioxo-2,3,4,5-tetrahydro-1,2,4-triazine-6-carboxamido)-phenylacetamido]-cephalosporanic acid, have antibiotic activity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **59133-55-0P**
(prepn. of)
RN 59133-55-0 USPATFULL
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[[(1,2-dihydro-2-oxo-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-8-oxo-, [6R-[6.alpha.,7.beta.(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

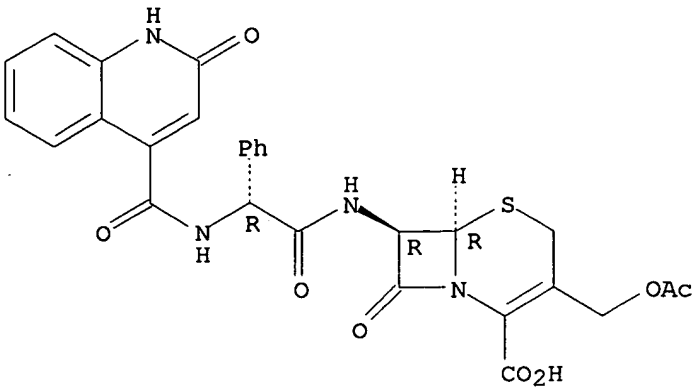


L12 ANSWER 2 OF 3 USPATFULL

AN 79:24260 USPATFULL
TI Cephalosporins having an .alpha.-acylaminoacetic acid side chain
IN Kocsis, Karoly, Basel, Switzerland
Peter, Heinrich, Binningen, Switzerland
Bickel, Hans, Binningen, Switzerland
PA Ciba-Geigy Corporation, Ardsley, NY, United States (U.S. corporation)
PI US 4154831 790515
AI US 77-789164 770420 (5)
RLI Division of Ser. No. US 75-576398, filed on 9 May 1975, now patented, Pat. No. US 4041161
PRAI CH 74-6494 740513
DT Utility
EXNAM Primary Examiner: Daus, Donald G.; Assistant Examiner: Wheeler, David E.
LREP Maitner, John J.
CLMN Number of Claims: 8
ECL Exemplary Claim: 1,4
DRWN No Drawings
LN.CNT 1119
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Compounds of the formula ##STR1## wherein R.sub.1 denotes optionally substituted phenyl, thienyl, furyl or 1,4-cyclohexadienyl, R.sub.2 represents a free carboxyl group or an esterified carboxyl group which can be split physiologically, R.sub.3 represents hydrogen, lower alkoxy or an optionally substituted methyl group and B represents an optionally substituted six-membered ring with 1 to 3 ring nitrogen atoms, which is bonded to the carbonyl group --C(.dbd.O)-- by one of its carbon atoms, the nitrogen atoms of a monocyclic six-membered ring having 2 nitrogen atoms being either adjacent or separated by two ring carbon atoms, and the salts of such compounds which have a salt-forming group, including the inner salts, for example the 7.beta.-[D(-)-.alpha.-(3,5-Dioxo-2,3,4,5-tetrahydro-1,2,4-triazine-6-carboxamido)-phenylacetamido]-cephalosporanic acid, have antibiotic activity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **59133-55-0P**
(prepn. of)
RN 59133-55-0 USPATFULL
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[[(1,2-dihydro-2-oxo-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-8-oxo-, [6R-[6.alpha.,7.beta.(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 3 OF 3 USPATFULL
AN 77:41963 USPATFULL
TI Cephalosporins having an .alpha.-acylaminoacetic acid side chain
IN Kocsis, Karoly, Basel, Switzerland
Peter, Heinrich, Binningen, Switzerland
Bickel, Hans, Binningen, Switzerland
PA Ciba-Geigy Corporation, Ardsley, NY, United States (U.S. corporation)
PI US 4041161 770809
AI US 75-576398 750509 (5)
PRAI CH 74-6494 740513
DT Utility
EXNAM Primary Examiner: Rizzo, Nicholas S.; Assistant Examiner: Wheeler, David E.
LREP Kolodny, Joseph G.; Maitner, John J.; Groeger, Theodore O.
CLMN Number of Claims: 6
ECL Exemplary Claim: 1,5
DRWN No Drawings
LN.CNT 1095
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Compounds of the formula ##STR1## wherein R.sub.1 denotes optionally substituted phenyl, thienyl, furyl or 1,4-cyclohexadienyl, R.sub.2 represents a free carboxyl group or an esterified carboxyl group which can be split physiologically, R.sub.3 represents hydrogen, lower akoxy or an optionally substituted methyl group and B represents an optionally substituted six-membered ring with 1 to 3 ring nitrogen atoms, which is bonded to the carbonyl group --C(.dbd.O)-- by one of its carbon atoms, the nitorgen atoms of a monocyclic six-membered ring having 2 nitrogen atoms being either adjacent or separated by two ring carbon atoms, and the salts of such compounds which have a salt-forming group, including the inner salts, for example the 7.beta.-[D(-)-.alpha.-(3,5-Dioxo-2,3,4,5-tetrahydro-1,2,4-triazine-6-carboxamido)-phenylacetamido]-cephalosporanic acid, have antibiotic activity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **59133-55-0P**
(prepn. of)
RN 59133-55-0 USPATFULL
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[[(1,2-dihydro-2-oxo-4-